# REPORT DOCUMENTATION PAGE

Form Approved
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1. AGENCY USE ONLY (Leave blank)	2. REPORT DATE	3. REPORT TYPE AND DATES COVERED
	March 2001	FINAL PROGRESS REPORT 4/97 to 12/00

4. TITLE AND SUBTITLE	5. FUNDING NUMBERS
Plasma Instability Driven Coherent Submillimeter Radiation Emitters	DAAG55-97-1-0021 ~~36603-PH~~

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7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)	8. PERFORMING ORGANIZATION REPORT NUMBER
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RECEIVED MAR 30 2001 BY

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)	10. SPONSORING/MONITORING AGENCY REPORT NUMBER
U.S. Army Research Office P.O. Box 12211 Research Triangle Park, NC 27709-2211	ARO 36603.12-PH

11. SUPPLEMENTARY NOTES

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12a. DISTRIBUTION/AVAILABILITY STATEMENT	12b. DISTRIBUTION CODE
Approved for public release; distribution unlimited.	A

13. ABSTRACT (Maximum 200 words)

We have introduced and studied lower dimensional solid state systems which could lead to experimental verification of current driven plasma instabilities, with potential device applications providing compact coherent Terahertz sources. A new approach, based on bounded systems in slab geometries (e.g. specially designed quantum well structures), shows that proper extraction and injection of carriers to maintain the desired nonequilibrium carrier distribution, leads to plasma instabilities in such systems. A complete theoretical framework was developed for transport and response of current driven non-equilibrium steady state systems. An interactive program was set up with the Tech. Univ. Vienna for experimental verification of these concepts. Quantitative agreement has been obtained for current voltage characteristics, validating the transport model. The predicted plasma and electromagnetic responses have been partially verified and will be further tested soon. We developed: energy level pair formalism for plasma modes and instabilities; self consistent formalism for non-equilibrium steady state systems; generalized RPA formalism for intersubband electron electron scattering including a magnetic field; intersubband electron-LO phonon scattering formalism; formuli for injection and extraction rates from transfer matrix; applications to various experiments for transport and response in quantum well structures.

14. SUBJECT TERMS		15. NUMBER OF PAGES
Current Driven Plasma Instabilities, Terahertz radiation sources, device applications, non equilibrium steady state transport and response		11
		16. PRICE CODE

17. SECURITY CLASSIFICATION OF REPORT	18. SECURITY CLASSIFICATION OF THIS PAGE	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT
UNCLASSIFIED	UNCLASSIFIED	UNCLASSIFIED	UL

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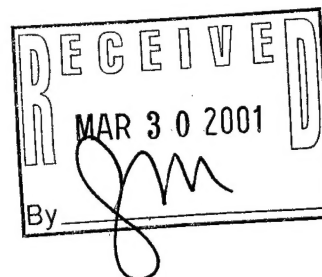
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REPORT TITLE: Plasma Instability Driven Coherent Submillimeter Radiation Emitters.

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Plasma Instability Driven
Coherent Submillimeter Radiation Emitters.

Final Progress Report

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March 2001

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1. Introduction

In this program we have introduced and studied systems which could lead to experimental verification of current driven plasma instabilities (CDPI) in lower dimensional solid state systems. Device applications based on this concept could lead to compact coherent sources in the Terahertz (submillimeter) range.

We have also set-up an interactive program for experimental verification of our results, with the Institute for Solid State Electronics at the Technical University of Vienna, Austria.

Several papers have been published based on the work in this program. This work also led to several other presentations, including several invited papers at international conferences.

The theoretical developments during this project, and the experimental results to date which already confirm our results, indicate that the main goal of this program, viz. the generation of (a) plasma instabilities, and (b) the ensuing electromagnetic radiation, in the THz range may be realized in the near future.

Section II provides a statement of the problem studied, section III summarizes the most important results and the last section lists the publications, and the participating scientific personnel.

II. Statement of the Problem

The basic problem investigated in this program was a study of CDPI in various lower dimensional (non-uniform) solid state systems, with the goal of developing a novel approach for generation or amplification of electromagnetic radiation in the millimeter and submillimeter ranges, with potential applications to a new class of THz devices.

The basic principle is to utilize the energy of a dc current passing through a plasma, which leads to a plasma-instability. The instability mechanism transfers the energy from the current to characteristic plasma waves, which grow in amplitude. These waves, in turn, can radiatively decay by interaction with a grating, or by dipole charge oscillations, or via specially shaped antennas, emitting electromagnetic radiation in the desired frequency range.

In earlier programs we had studied high mobility, lower dimensional, *uniform* systems as the solid state media for achieving CDPI. The required drift velocities had to be of the order of, or greater than the Fermi velocities. Subsequently we examined the possibilities of CDPI in *periodically modulated systems*. These require significantly lower drift velocities to achieve CDPI, bringing them within reach of experimental verification.

In the present program, we have developed a new approach based on *bounded systems* in slab geometries (e.g. specially designed quantum well structures). In such systems, with proper extraction and injection of carriers to maintain the desired nonequilibrium carrier distribution, we show that strong plasma instabilities will develop. Such systems could then lead to experimental verification of this concept and future device applications. We describe in detail in the next section the theoretical framework we have developed for proper description of these non-equilibrium, current driven, steady state systems.

An interactive collaborative program has been set-up with the Vienna group to achieve experimental verification of these ideas. Several quantum well structures have been grown according to our designs, and as discussed below, significant agreement between experiment and theory has been demonstrated for their I-V characteristics. Also, emitted radiation has been observed at frequencies predicted theoretically.

III. Main Results.

There were nine major areas covered in this program. We summarize below the main results:

1. Plasma modes in modulated 1D systems

We have studied the normal modes of quasi-1D periodically modulated plasmas, including their damping due to the periodicity induced single particle excitations. This latter aspect has not been discussed in the literature. We also obtain the zone boundary plasmons of this system, similar to those obtained for higher dimensional systems with periodic modulation.

Part of this work was presented at the 1998 APS March Meeting (Bull. Amer. Phys. Soc. 43, 869, 1998). This topic also constitutes a part of a Ph.D. thesis completed under our supervision: H. Xie, "Current Driven Plasma Instability in Lower Dimensional Solid State Systems", Ph.D. Thesis, Boston College, December 1997.

2. Energy level pair formalism for plasma modes and instabilities

Our calculations of instabilities are done using the random phase approximation (RPA), with a self-consistent non-equilibrium steady state. While the full computer programs give us the results for any specific scenario that we desire, the underlying simplicity (if any) does not necessarily come through in a computer calculation. A new formalism that we have developed (energy level pair formalism) makes it possible to see the underlying simplicity of the essential process that gives rise to the plasma instability. The entire plasma dynamics is considered in terms of all possible energy level pairs amongst

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which transitions can occur. It turns out that an instability occurs when the (single particle) down transition frequency ($\approx \Omega$), for a pair, slightly exceeds the up transition frequency ($\approx \omega$) of another pair. The depolarization shift effects, which reduce the down frequency to Ω', and increase the up frequency to ω', bring them into resonance ($\Omega' = \omega'$). This inter-pair interaction at resonance is what generates plasma instabilities in all cases we have studied. Essentially the plasmon emitted in the down transition gets absorbed through the up transition, thus coupling the dynamics of the populations of the two pairs at resonance. This built-in feedback process generates the plasma instability. This microscopic understanding of the essential phenomenon for our program has been extremely helpful in designing appropriate structures for generating the instability. This work was initially presented as an invited paper at the 20th International Workshop on Condensed Matter Theory, Pune, India, December 1996 and is now published as a detailed paper (Ref. 1).

3. Full self-consistent formalism.

A fully self-consistent computational scheme for obtaining the non-equilibrium steady state for various quantum well structures under bias has been developed. This formalism goes far beyond the approach used in our previous work. Now the eigenstates are determined by the Schroedinger-Poisson scheme, and the subband populations are determined by rate balance equations for each subband. These balance equations require various transport rates. The inter-subband transfer rates via electron-electron interactions are obtained through a RPA self-energy calculation. The inter-subband electron-LO phonon transfer rates are obtained through a matrix elements approach. The injection-extraction rates are obtained by determining the transfer matrix for the structure for complex energies. These three rate calculations are described in detail in the next section. The self-consistent solution at any given bias is obtained when the input subband populations used for determining the non-equilibrium steady state agree with the output populations obtained through the rate balance equations.

The feasibility of plasma instability for the resulting non-equilibrium steady state is examined for each bias through a response calculation. The I-V curves and the domains of instability (as a function of bias) are obtained for any structure. Full spectral response is also calculated, and is useful for direct diagnosis of the properties of a given structure. This formalism, which is fully quantum mechanical, applies to structures without internal doping, and is thus ideal for the design of the current generation of structures.

This scheme was presented at the 3rd International Workshop on MBE-Growth Physics and Technology, Warsaw, May 1999, and the corresponding paper has appeared in the journal Thin Solid Films (Ref.2). A complete version of the formalism was presented at the 5th International ITQW'99 Conference, Bad Ischl, Austria, September 1999, and the corresponding paper has appeared in Physica E (Ref.3).

4. Formalisms for various transport rates

a. Generalized RPA formalism for inter-subband electron-electron scattering.

We have developed a comprehensive formalism for inter-subband scattering due to the electron-electron interactions, based on the calculation of the self-energy of the carriers in the system under RPA. It can be shown that the so-called Auger process constitutes only the first bubble diagram in an infinite series which is summable under RPA. This formalism properly takes into account all the inter-subband transitions involving carrier-carrier interactions, including collective effects involving plasmon creation and absorption. The formalism was initially developed for zero temperature, and then generalized for finite temperature equilibrium systems, using Matsubara formalism. The latter formulation was further generalized to non-equilibrium distributions.

Our formalism explains quantitatively the diverse experimental results of N. Heyman, et al., Phys. Rev. Lett. 74, 2682(1995) and Physica E2, 195 (1998), and M. Hartig et al., Phys. Rev. Lett. 80, 1940(1998). Our work was presented at the 5th International ITQW'99 Conference, Bad Ischl, Austria, September 1999, and the corresponding paper has appeared in Physica E (Ref.4). A more detailed paper has been published in Phys. Rev. B. (Ref.5).

b. Formalism for inter-subband electron-LO phonon scattering rates for quantum well systems.

While the electron-LO phonon scattering formalism for bulk system is textbook material, it requires appropriate adaptation for quantum well structures (systems confined in one dimension by arbitrary potential, and open in the other two dimensions). This has been carried out, and cast in a computable form for arbitrary quantum well structures. The results were tested against other calculations in the literature (e.g. Harrison, et. al. In Proceedings of IEEE Sixth International Conference on Terahertz Electronics, pp. 74-78

and 223-226, IEEE Catalog No. 98 EX 171, 1998), and then applied to our systems. This new component of our calculations has been fully integrated into our self-consistent program. The main finding is that the electron-LO phonon scattering rates depend very sensitively on the shape and asymmetry of the quantum well structure. Due to phase space limitations, these rates are much lower than for bulk material.

c. Injection and extraction rates.

Injection and extraction rates α_j and β_j are determined by the transfer matrx for complex energies. The complex energy pole of the transmission coefficient determines the total width ($\alpha_j + \beta_j$) of the quasi bound energy level. The ratio β_j / α_j is related to a matrix element of the transfer matrix. These two relations determine α_j and β_j for any given quantum well structure. A brief summary of the method is given in our Ref.3.

5. Comparison of theory and experiments

Quantitative comparison of our theoretical predictions for the differential conductance profile for the structures g205 and g301 with the experimental results was reported in JAP 85, 3708, 1999 (Ref.6). Good agreement was obtained.

Quantitative comparison of our theoretical predictions for the emission of radiation for the structures g205 and g301 with the experimental results was reported in APL 75, 1685, 1999 (Ref.7). Good agreement was obtained.

Both of these studies showed that the heavy doping of the active region in these structures produced subband level broadening, and corresponding emission line broadening. This can be avoided by designing structures without any doping in the active region. Such structures were designed and grown.

Two structures were designed (g389 and g390) without any doping in the active region. Since doping in the previous structures was considered effective in retaining more electrons in the active region, we simulated this effect in these new structures without any doping through a parabolic grading of the aluminum content in the active region. This produces a parabolic confining potential similar to that of a doped structure, without introducing the high collisionality of the doped structures. While g389 had a pocket region as in the case of the previous structures, g390 was designed without the pocket, for comparison purposes. Both structures had single barriers for injection and extraction.

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These structures were grown, their I-V characteristics were measured, and compared with the theoretical predictions. Quantitative agreement was obtained for the magnitude of the current, as well as, the differential conductance. As expected, g389 showed more pronounced features under reverse bias. These results were presented at the International Conference EUROPTO 1999, Terahertz Spectroscopy and Applications, Munich, Germany, June 1999, and published in the Conference Proceedings, SPIE vol.3828, pp. 151-159 (1999), (Ref.8).

The next structure was designed so as to achieve population inversion, and emit radiation in the THz range. This structure was similar to g301, except that it had no doping in the active region, and a parabolic grading replaced the plateau region. The proposed doping density outside the active region was 2×10^{18} cm^{-3}. The I-V, as well as radiation response characteristics were calculated for this structure. The strongest plasma instability for this structure had a growth rate of 0.68 meV. The corresponding structure was grown (g428), but the outside doping density, unfortunately, was only 1.5×10^{18} cm^{-3}. Thus our original calculations would not apply to this structure. We recalculated the properties of this structure with the lower density. We found very good agreement for the current as well as the differential conductance. Our calculations showed a very weak instability ($\gamma = 0.2$ meV) for g428, not sufficient to overcome the residual interface and Al concentration change related collisional losses. Emission experiments for g428 showed no emission of radiation, as is to be expected due to low electron density.

A structure, with higher doping density outside the active region (2.4×10^{18} cm^{-3}), has now been grown (g494) and shows very good agreement with the calculated I-V characteristics. Emission measurements will take place in the near future and will be compared with theoretical predictions, which show high growth rates for instabilities in excess of 1 meV.

6. Non-linear dynamical oscillations in an inhomogeneous bounded structure

We showed, that even without population inversion, if in addition to a plasmon bath there is a region where a dynamic charge inhomogeneity can develop, this could lead to non-linear dynamical oscillations of the inhomogeneous bounded plasma. Essentially, the charge inhomogeneity adds an imaginary component to the plasma susceptibility, leading to a plasma instability. The large amplitude oscillations saturate in a limit cycle behavior. Specific structures were proposed where this phenomenon may be realized. Parameters can be adjusted to utilize this phenomenon to generate THz radiation. A

preliminary version was presented at the International Conference EUROPTO 1999, Terahertz Spectroscopy and Applications, Munich, Germany, June 1999, and published in the Conference Proceedings, SPIE vol.3828, pp. 151-159 (1999), (Ref.8).

7. Inter-subband THz emission in current driven parabolic quantum well cascade structures.

In a recent experiment at UCSB, a single peak emission of THz radiation was observed from two current driven cascade structures, single segment of which consists of a parabolically graded quantum well. In one version of the structure, the parabolic regions are separated by simple barriers, and in another version by "chirped" short superlattices. The superlattice acts as a narrow band filter of electrons travelling from one parabolic region to another

We calculated the emission spectra for these structures using our formalism, and the observed radiation frequency in each case was in agreement with the calculated response. A similar sample was grown in Vienna, with a slight modification of the parabolic region. We also calculated the response for this structure, and predicted two emission peaks, which are in agreement with the experimental results. Our calculations show that the lower frequency peak arises from the superlattice barriers.

8. Effects of magnetic field on electron-electron intersubband scattering rates in quantum wells.

We extended the calculations for inter-subband relaxation processes due to the electron-electron scattering in a quantum well structure, to include a magnetic field. We find that the scattering rate is peaked at two possible sets of arrangements of the Landau levels (LL) of the two subbands of interest. The first set occurs when the LL of both subbands align, and the other when the LL misalign, so that the LL of one subband lie exactly in the middle between those of the other subband. Experiments on various quantum cascade structures show that the misaligned set of transitions is completely suppressed. From our calculations this implies that there is *no* population inversion in those structures. Since this effect is observable in I-V characteristics, this provides a simple diagnostics of the population inversion in various quantum well structures.

9. Other Topics

In addition to these activities, we published a paper on "Collective vs. Individual Dot Response of Quantum Dot Ensambles", presented at the Strongly Coupled Coulomb Systems Conference, August 1997, Ref.9. This work has a bearing on the effect of inhomogeneity across the mesa plane in our structures.

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1. P. Bakshi and K. Kempa, "Mathematical Signatures of Plasma Instabilities in Low Dimensional Systems," *Condensed Matter Theories*, Vol. 12, 399-412 (1997). Eds. J. Clark and P. Panat, Nova Science Publishers, New York.

2. K. Kempa, P. Bakshi, "Computer simulations of the Transport and Electromagnetic properties of MBE grown quantum structures", Thin Solid Films 367, 295-298 (2000).

3. P. Bakshi, K. Kempa, "Intersubband plasmon emission based THz Lasers", Physica E 7, 63-68 (2000).

4. K. Kempa, P. Bakshi, J. R. Engelbrecht, and Y. Zhou, "Intersubband relaxation due to electron-electron scattering in quantum well structures", Physica E 7, 225-228 (2000).

5. K. Kempa, P. Bakshi, J. R. Engelbrecht, and Y. Zhou, "Intersubband electron transitions due to electron-electron interactions in quantum well structures", Phys. Rev. B 61, 11083-1187 (2000).

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9. P. Bakshi and K. Kempa, "Collective vs. Individual Dot Response of Quantum Dot Ensembles," *Strongly Coupled Coulomb Systems*, pp 503-507, (1998), ed. G. Kalman et al, Plenum Press.

IV. Publications and Personnel.

a) Publications

1. P. Bakshi and K. Kempa, "Mathematical Signatures of Plasma Instabilities in Low Dimensional Systems," *Condensed Matter Theories*, Vol. 12, 399-412 (1997). Eds. J. Clark and P. Panat, Nova Science Publishers, New York

2. H. Xie, "Current Driven Plasma Instability in Lower Dimensional Solid State Systems," Ph.D. thesis, Boston College (1997).

3. P. Bakshi and K. Kempa, "Collective vs. Individual Dot Response of Quantum Dot Ensembles," *Strongly Coupled Coulomb Systems*, pp 503-507, (1998), ed. G. Kalman et al, Plenum Press.

4. K. Kempa, P. Bakshi, C. Du, G. Feng, A. Scorupsky, G. Strasser, C. Rauch, K. Unterrainer and E. Gornik, "Towards Stimulated Generation of Coherent Plasmons in Nano-structures," J. Appl. Phys. 85,3708-3712 (1999).

5. P. Bakshi, K. Kempa, A. Scorupsky, C. Du, G. Feng, R. Zobel, G. Strasser, C. Rauch, Ch. Pacher, K. Unterrainer and E. Gornik, "Plasmon based THz emission from quantum well structures", Appl. Phys. Letts. 75, 1685-1687 (1999).

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8. K. Kempa, P. Bakshi, J. R. Engelbrecht, and Y. Zhou, "Intersubband relaxation due to electron-electron scattering in quantum well structures", Physica E 7, 225-228 (2000).

9. K. Kempa, P. Bakshi, J. R. Engelbrecht, and Y. Zhou, "Intersubband electron transitions due to electron-electron interactions in quantum well structures", Phys. Rev. B 61, 11083-1187 (2000).

10. K. Kempa, P. Bakshi, "Computer simulations of the transport and electromagnetic properties of MBE grown quantum structures", Thin Solid Films 367, 295-298 (2000).

b) Personnel

1.   Prof. P. Bakshi (Faculty), Principal Investigator
2.   Prof. K. Kempa (Faculty), Principal Investigator
3.   H. Xie (Graduate Student), Research Assistant
4.   A. Scorupsky (Graduate Student), Research Assistant
5.   G. Feng (Graduate Student), Research Assistant
6.   Dr. C. Du, Research Scientist

c) Degree earned.

H. Xie: Ph.D., Boston College (1997)

d) Reportable inventions.

Invention Disclosure "A method and apparatus for generating Terahertz-Gigahertz electromagnetic radiation", by K. Kempa and P. Bakshi, was filed with the Office of Research Administration, Boston College, December 1998.